

Small-angle scattering of neutrons on large scale inhomogeneities in refraction range

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The small-angle scattering of neutrons on large scale inhomogeneities of two-component systems in refraction range is considered. We supposed, that neutrons acquire phase shifts describing by the Gaussian distribution function. It is shown that the average cross section of scattering contains two contributions. The first contribution describes the diffraction and in the asymptotic limit of large transfer momentum this contribution is proportional to $q^{-\Delta}$, where $2 \leq \Delta \leq 4$. The second contribution is similar to the Fraunhofer diffraction, which in the asymptotic limit of large transfer momentum is proportional to q^{-3} .

I. INTRODUCTION

Small-angle neutrons scattering is the powerful method to study large scale inhomogeneities of different structures in condensed matter¹⁻⁵. Usually, experimental data are interpreted within the Born approximation. However, when neutrons are scattered on large scale inhomogeneities refraction processes can give a significant contribution in the scattering cross section. The amplitude of small-angle scattering of neutrons under propagation through an inhomogeneity is defined by the phase shift $\delta(\boldsymbol{\rho})$, where $\boldsymbol{\rho}$ is a transfer momentum perpendicular to the direction of the neutron beam (see for example⁶). In the case, when $\delta(\boldsymbol{\rho}) \ll 1$, the Born approximation is valid, in the opposite case, when $\delta(\boldsymbol{\rho}) \gg 1$, refraction effects became considerable and the Born approximation is not applicable¹.

It is well known² that for two-component system having inhomogeneities with smooth boundaries the intensity of scattering $I(\mathbf{q})$ falls off with increase of the transfer momentum \mathbf{q} according to the Porod law q^{-4} . However in most cases the surface dividing phases of the system cannot be considered as smooth. In particular, the scattering of neutrons in Ising-like magnetic systems in an external magnetic field^{3,7-11} occurs on domain walls, with a surface strongly differs from a smooth plane. The scattering on two-component systems with rough interfaces of phases is investigated in detail within the Born approximation^{3,4}. It was shown that the intensity of scattering has the contribution, which is described by the power function of the transfer momentum with the exponent less than 4. Deviations from the Porod law take place also for scattering on fractal structures¹². These results agree well with a lot of experimental data. It is necessary to emphasize, that in this case a refraction processes are absolutely omitted from consideration. However these processes can be very important for the studying of neutron scattering in systems with large scale

inhomogeneities when the Born approximation becomes inapplicable.

In the theory of the scattering on large scale spherical inhomogeneities it is well known¹³ that for the case of an inapplicability of the Born approximation the amplitude of scattering consists of three terms (diffraction, refraction and so-called residual term) in correspondence with the expression for the forward scattering amplitude by spherical inhomogeneities (see for example⁶). However, we don't know the precise expression for residual term unlike the diffraction and refraction contribution to the scattering amplitude, but we can to expand this expression in power series of $1/\alpha$ (where α is the Born parameter) and to get approximate estimation only. According to this fact the range where $\alpha \gg 1$ was called refraction, and the range $\alpha \ll 1$ was called diffraction correspondingly. Recently¹⁴ for the residual term of the amplitude of the scattering by spherical inhomogeneities the precise expression was obtained. This expression contains special functions, the arguments of which have two dimensionless parameters: the Born parameter and the product qR , where R is a radius of the inhomogeneity. In this case, the transition of the amplitude of scattering from the diffraction range to the refraction occurs not for $\alpha \sim 1$ but for $\alpha \sim qR$. It worth to point, that in the asymptotic limit $qR \gg 1$ the diffraction range "analytically continue" in the area prohibited for it $\alpha > 1$ and, correspondingly, the refraction range is shifted.

The influence of the refraction processes in the multiple neutron scattering on large scale inhomogeneities is especially important^{15,16}. According to the general theory of scattering¹⁷ the intensity of the multiple scattering is completely determined by single scattering cross section. Usually, it is considered the case, when the dominating contribution to the cross section of single scattering introduces the diffraction range of scattering¹⁸. In this case the cross section of single scattering on spherical inhomogeneities in the limit $qR \gg 1$ is described

by the function $(qR)^{-4}$. In the refraction range in the same limit $qR \gg 1$ the single cross section of scattering contains terms $(qR)^{-3}$ and $(qR)^{-4}$ due to the existence of the refraction term¹. Therefore for the case, when the refraction range gives the dominant contribution to the cross section of single scattering, the change of the intensity of multiple scattering take place due to an appearance of new asymptotic behavior of single scattering cross section¹⁶.

The main aim of this work is to study just refraction processes in systems where the declination of the scattering intensity from the Porod law is observed. Next such systems we call the fractal systems. We do not know the amplitude of scattering in the refraction range when the scattering occurs in the fractal medium unlike of scattering on spherical inhomogeneities. However the amplitude of scattering in the refraction range can be restored by the known amplitude of the Born approximation if we use the formal expression of phase shift by a Fourier transform of the Born amplitude of scattering on transfer momentum. It is worth especially to emphasize, that there is no necessity to assume the smallness of the Born parameter of the theory of scattering in this case. Hereinafter we interested by systems with known cross section instead of the scattering amplitude in the Born approximation. The Born cross section is presented by the correlation function of local fluctuations of the Born scattering amplitude³ that is local fluctuations of phase shifts. The main assumption of our work is that we average the correlation function according to the Gaussian function that is we assume that phase shifts are Gaussian random variables and mean-square fluctuations of phase shifts coincide with the Born scattering cross section. Thus the correlation functions are easily calculated and the refraction part of the cross section can be selected. The choice a distribution function by the Gaussian function for the description of the refraction range gives the right expression for the well known Babinet principle with exponential accuracy. This allows to hope that results obtaining in this work are correct in this range of scattering.

II. SCATTERING ON TWO-COMPONENT FRACTAL SYSTEMS IN BORN APPROXIMATION

Within the limit of small phase shifts $\delta(\rho) \ll 1$, the single scattering is described by the Born approximation. In this limit the scattering intensity $I(\mathbf{q})$ is presented by the correlation function of density fluctuations of scattering objects $\gamma(\rho)^{1-4}$. If for two-component systems the surface is smooth then the Porod law for the intensity² occurs, $I(q) \sim q^{-4}$, in the limit of large transfer momenta q . If the surface is rough it was obtained by two various methods^{3,4} that the correction to the Porod law can be written as

$$\frac{d\sigma}{d\Omega} \sim \frac{A_1}{q^4} + \frac{A_2}{q^{x+3}}, \quad (1)$$

where x , ($0 \leq x \leq 1$) is the parameter describing roughness of surface⁸. It is necessary to note that in the case when the second term in Eq. (1) dominates, the Eq. (1) describes the scattering cross section in fractal medium¹². We remind that for scattering on volume fractals the scattering cross section within the limit of large transfer momenta is proportional to q^{-D_v} , where $D_v < 3$, for scattering on surface fractals the cross section is proportional to $q^{-(6-D_s)}$, where $D_s < 3$ and at last for a scattering on critical fluctuations the cross section is proportional to q^{-2} . Thus the general expression of the scattering cross section covering all these particular cases can be described by the equation $q^{-\Delta}$, where $2 \leq \Delta \leq 4$.

III. THE CROSS SECTION IN EIKONAL APPROXIMATION

Now we attempt to go beyond the Born case and to study refraction processes of small-angle scattering of neutrons in fractal systems using the eikonal approximation^{6,17}. In this case it supposed, that the energy of incident particles is a lot of more then the potential energy of scattering and the amplitude is written as

$$f(\mathbf{q}) = -\frac{ik}{2\pi} \int (\exp[2i\delta(\rho)] - 1) \exp(-i\mathbf{q}\rho) d^2\rho, \quad (2)$$

where \mathbf{q} is the two-dimensional transfer momentum lying in the plane perpendicular to the beam of neutrons with momentum k , $\delta(\rho)$ is the phase shift. The cross section is defined as

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f(\mathbf{q})|^2 = \left(\frac{k}{2\pi}\right)^2 \int d^2\rho d^2\rho' \exp(-i\mathbf{q}(\rho - \rho')) \times \\ &\quad (S(\rho) - 1)(S^*(\rho') - 1) \\ &= \left(\frac{k}{2\pi}\right)^2 \int d^2\rho \exp(-i\mathbf{q}\rho) \gamma'(\rho), \end{aligned} \quad (3)$$

here we define the function

$$\gamma'(\rho) = \int d^2\rho' (S(\rho' + \rho) - 1)(S^*(\rho') - 1), \quad (4)$$

and also

$$S(\rho) = \exp 2i\delta(\rho), \quad \delta(\rho) = -\frac{1}{2\hbar v} \int U(\rho, z) dz, \quad (5)$$

$U(\rho, z)$ is the scattering potential, and v is the velocity of particles. For small phase shifts the exponential functions in Eqs. (4, 5) can be expand in power series and the correlation function $\gamma'(\rho)$ is transformed to the $\gamma(\rho)$ of the Born approximation.

It is easy to see from Eq. (3) that the scattering cross section is determined by the dependence of phase shift δ

on the impact parameter ρ . This dependence can be found by the known Born scattering amplitude. It should be noted that formally the phase shift is the Fourier transform of the scattering amplitude in the Born approximation

$$\delta(\rho) = \frac{\pi}{k} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} f_B(\mathbf{q}) \exp(i\mathbf{q}\rho). \quad (6)$$

In other words instead of using the direct definition of the phase shift by the scattering potential Eq. (5) it can be more suitable sometimes (for example at the scattering on spherical inhomogeneities or superconducting vortex lines) to find the phase shift by the known Born amplitude. Besides this method allows in the eikonal approximation analytically to continue the phase shift to the region of large Born parameters since the formal equation (6) does not assume a smallness of this parameter in the scattering theory.

Unfortunately we known the Born cross section but don't know the Born amplitude for fractal medium. However the cross section is represented by the appropriate density fluctuations correlation function (see for example¹⁹). To present the cross section in refraction range by the correlation function of density fluctuations we assume that phase shift is a local random variable which in the primary approximation can be described by the Gaussian distribution. Define the Gaussian distribution function of phase shifts $\delta_{\mathbf{q}}$ in the momentum representation $\delta_{\mathbf{q}}$ as

$$P(\delta_{\mathbf{q}}) = \frac{1}{Z} \exp\left(-\frac{|\delta_{\mathbf{q}}|^2}{2\langle|\delta_{\mathbf{q}}|^2\rangle}\right), \quad (7)$$

where Z is the partition function written by the functional integral

$$Z = \int \mathcal{D}\delta_{\mathbf{q}} \exp\left(-\frac{|\delta_{\mathbf{q}}|^2}{2\langle|\delta_{\mathbf{q}}|^2\rangle}\right). \quad (8)$$

The mean-square fluctuation of phase shifts defines the Born cross section of scattering in the form

$$\langle|\delta_{\mathbf{q}}|^2\rangle = \frac{1}{S} \left(\frac{\pi}{k}\right)^2 \left\langle \frac{d\sigma}{d\Omega} \right\rangle_B. \quad (9)$$

Here S is the geometrical cross section of inhomogeneity and $\langle \frac{d\sigma}{d\Omega} \rangle_B$ is the Born cross section of single scattering. The angle brackets mean the average over the Gaussian fluctuations.

For the cross section we have

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \left(\frac{k}{2\pi}\right)^2 \int d^2 \rho d^2 \rho' \exp(-i\mathbf{q}(\rho - \rho')) \times \langle (\exp(2i\delta(\rho)) - 1)(\exp(-2i\delta(\rho')) - 1) \rangle. \quad (10)$$

Calculating the mean value of exponential functions of random variables distributed according to the Gaussian function¹⁹, we rewrite expression Eq. (10) as

$$\begin{aligned} \left\langle \frac{d\sigma}{d\Omega} \right\rangle = & \left(\frac{k}{2\pi}\right)^2 \int d^2 \rho d^2 \rho' \exp(-i\mathbf{q}(\rho - \rho')) \times \\ & \left\{ \exp\left[-\frac{4}{S} \left(\frac{\pi}{k}\right)^2 \int \frac{d^2 \mathbf{q}'}{(2\pi)^2} \left\langle \frac{d\sigma}{d\Omega} \right\rangle_B \times \right. \right. \\ & \left. \left. (1 - \exp(i\mathbf{q}'(\rho - \rho')))\right] \right. \\ & \left. - 2 \exp\left(-\frac{2}{S} \left(\frac{\pi}{k}\right)^2 \int \frac{d^2 \mathbf{q}'}{(2\pi)^2} \left\langle \frac{d\sigma}{d\Omega} \right\rangle_B\right) + 1 \right\}. \quad (11) \end{aligned}$$

Expanding of exponents in power series in Eq. (11) leads to the Born cross section that corresponds to transition in the diffraction range of scattering.

It is conveniently to define the function $\sigma_B(\rho)$ as

$$\begin{aligned} \sigma_B(\rho) &= \frac{1}{k^2} \int d^2 \mathbf{q} \left\langle \frac{d\sigma}{d\Omega} \right\rangle \exp(i\mathbf{q}\rho), \\ \sigma_B(\rho = 0) &= \sigma_B(0). \end{aligned} \quad (12)$$

Here $\sigma_B(0)$ is the total Born cross section where the magnitude of the Born parameter is large in refraction range of scattering. Substituting Eq. (12) in Eq. (11) we have

$$\begin{aligned} \left\langle \frac{d\sigma}{d\Omega} \right\rangle = & \frac{k^2}{2\pi} S \int d\rho \rho J_0(q\rho) \exp\left(-\frac{\sigma_B(0)}{S} \zeta(\rho)\right) \\ & + \left(1 - 2 \exp\left(-\frac{\sigma_B(0)}{2S}\right)\right) \left(\frac{k\xi}{q}\right)^2 J_1^2(q\xi), \end{aligned} \quad (13)$$

where we define the function

$$\zeta(\rho) = 1 - \frac{\sigma_B(\rho)}{\sigma_B(0)}. \quad (14)$$

The first term in Eq. (13) is the known expression for the scattering intensity in the theory of multiple neutron scattering¹⁸. It is necessary to emphasize, that in this case the value of $\sigma_B(0)/S$ in refraction range became large in contrast with unit more just due to that in the equation for $\sigma_B(0)$ the smallness of the Born parameter does not assume. Calculating the integral in the last term in Eq. (13) we assume that a size of fractal objects under scattering is limited by correlation length ξ due to average by all chaotic orientations of the fractal object of course. It is worth to note that the obtained expression for the second term is analogous to the Fraunhofer diffraction on the round hole²⁰. In the asymptotic limit of large transfer momenta the Fraunhofer diffraction is described by the function q^{-3} . For an arbitrary fractal the result of the calculation of this integral would be similar of the Fraunhofer diffraction on the hole which has a form corresponding to this fractal.

Calculating the integral Eq. (11) over the two-dimensional vector q , we have the total cross section

$$\sigma = \int d\mathbf{q} \left\langle \frac{d\sigma}{d\Omega} \right\rangle = 2S \left[1 - \exp\left(-\frac{\sigma_B(0)}{2S}\right) \right] \quad (15)$$

The ratio $\sigma_B(0)/2S$ is proportional to the square of the Born parameter. The Eq. (15) can be rewritten as the

equation in the Born approximation if the Born parameter is small in comparison with unit. The total cross section is equal to the double geometrical section in the case of the large Born parameter. This result is in complete correspondence with the Babinet principle. According to this principle the total cross section is determined by a double cross section of an absorption^{6,20}.

In general the differential cross section of scattering in the Born approximation can be presented as

$$\langle \frac{d\sigma}{d\Omega} \rangle_B = Aq^{-\Delta} f_{\Delta}(q\xi), \quad (16)$$

where A is a constant. Δ is a some parameter in the interval ($2 \leq \Delta \leq 4$). The function $f_{\Delta}(q\xi)$ within the limit of a large $q\xi$ can be replaced by unit but for the case of small transfer momentum it ensures not singular behavior for the scattering cross section. Substituting Eq. (16) in Eq. (14) and making the substitution of a variable $\lambda = k\rho$, we get

$$\zeta(\lambda) = \frac{\int_0^{\infty} dx x^{-\Delta+1} [1 - J_0(\vartheta_0 \lambda x)] f_{\Delta}(x)}{\int_0^{\infty} dx x^{-\Delta+1} f_{\Delta}(x)}, \quad (17)$$

where $\vartheta_0 = 1/k\xi$.

Since the main contribution to the integral of Eq. (13) is given by small λ , we can replace $f_{\Delta}(x)$ by unit in the numerator of Eq. (17). As a result for $2 < \Delta < 4$ we have a known integral, which results to

$$\zeta(\lambda) = (\vartheta_0 \lambda / 2)^{\Delta-2} / F_{\Delta}, \quad (18)$$

where

$$F_{\Delta} = \frac{(\Delta - 2)\Gamma(\Delta/2)}{\Gamma(2 - \Delta/2)} \int_0^{\infty} dx x^{1-\Delta} f_{\Delta}(x). \quad (19)$$

The equation (13) is:

$$\begin{aligned} \langle \frac{d\sigma}{d\Omega} \rangle = & \frac{S}{2\pi} \frac{k^2}{q^2} \int_0^{\infty} dx x J_0(x) \exp \left[- \left(\frac{\sigma_B}{SF_{\Delta}} \right) \left(\frac{x}{2q\xi} \right)^{\Delta-2} \right] \\ & + \left[1 - 2 \exp \left(- \frac{\sigma_B}{2S} \right) \right] \left(\frac{k\xi}{q} \right)^2 J_1^2(q\xi). \end{aligned} \quad (20)$$

Here we transformed the first term in Eq. (20) similar to the known equation²¹, therefore it is possible to use known result¹⁷ that in asymptotic limit the intensity of multiple scattering coincide with the intensity of single scattering. In this case the single scattering intensity is defined by Eq. (16). The refraction term (which in asymptotic limit is proportional to q^{-3}), can become the main one in the intensity depending on a kind of the law for the intensity of a single scattering. Really, for $3 < \Delta < 4$ exists a range of values of transfer momentum where in the intensity dominates the Fraunhofer diffraction with asymptotic dependence q^{-3} . The range $3 < \Delta < 4$ corresponds to the scattering on surface fractals when the parameter x in the Eq. (1) change in limits $0 < x < 1$. In the other limits $2 < \Delta < 3$, which

corresponds to the scattering on a volume fractals, the Fraunhofer diffraction already does not render essential influence to the intensity of scattering already.

In the specific case $\Delta = 4$ the cross section Eq. (16) is described by the Porod law. This case is well investigated in the theory of multiple scattering on spherical inhomogeneities^{18,15}. Here the intensity of multiple scattering transforms in the intensity of single scattering in asymptotic limit of large transfer momentum too¹⁷. The analysis of this case begins with the equation (13), where for the first term we can use the result of the multiple scattering theory again. This result shows, that in an asymptotic limit the intensity of multiple scattering is determined by the cross section in the Born approximation q^{-4} . Therefore, for this case, as well as for previous, it is possible to assert, that the cross section of small-angle neutron scattering in refraction range in fractal medium with a parameter ($x = 1$ in the equation (1)) is described by the Fraunhofer diffraction.

The refraction term does not render essential influence to the intensity of scattering in the other special case, when $\Delta = 2$. This case describes the scattering on critical fluctuations. Here also it is necessary to analyze the Eq. (13) and we must for the first term to use the result of the multiple scattering theory. This multiple scattering theory on critical fluctuations is considered in Ref.¹⁸, where the dependence of the multiple scattering intensity on the transfer momentum in the asymptotic limit of large momenta was found. These functions give the predominant contribution in comparison with the refraction term.

IV. CONCLUSIONS

Thus at studying of the small-angle neutron scattering in fractal medium in the refraction range (that is for the case when the Born parameter of the theory of scattering is not small) it is necessary for the single cross section to take into account the contribution proportional q^{-3} within the large transfer momentum limit which is similar to the Fraunhofer diffraction. Depending on the value of the exponent Δ of the single scattering cross section in the Born approximation the averaged correlation function over the Gaussian random variables in refraction range gives a very small contribution to the cross section for $\Delta > 3$. In the opposite case the Fraunhofer diffraction is negligible.

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